TP computing lab - Integrating the 1D stationary Schrödinger equation

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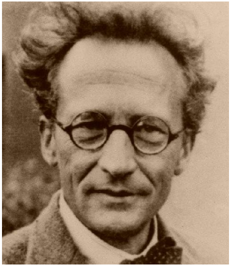


The time-independent (stationary) Schrödinger equation is given by

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x), \qquad (1)$$

$\psi(x)$ is the wavefunction of the particle,
E the corresponding energy,
$\hbar$ is Planck's constant divided by 2π,
m the mass of the particle,
$V(x)$ the potential under consideration.

- Eigenvalue problem: Solutions that satisfy boundary conditions ($\psi(x \to \pm\infty)$=0) only exist for certain discrete values of E.
- Can be solved analytically for a few potentials such as harmonic potential ($V(x) \propto x^2$) or the infinite square well.

Aims of the computing lab

- Use shooting/matching method to find the Eigenstates and corresponding energy Eigenvalues numerically for the infinite square well
- How accurate can we get this? $\rightarrow$ Compare with analytic solution.
- Use numerical algorithm to find Eigenstates of a more complicated potential.
- Check orthogonality of the Eigenstates.

Some general remarks on Schrödinger equation

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x),$$

- If $\psi(x)$ is a solution, then $C \cdot \psi(x)$ is also a solution.
- The probability distribution function is given by $P(x) = \psi^*(x)\psi(x)$. Need to normalize such that $\int_{-\infty}^{\infty} \psi^*(x)\psi(x) = 1$
- Whenever the potential $V(x)$ has even parity (i.e symmetric) then the solutions have either even or odd (=antisymmetric) parity.
- The normalized eigenstates are orthonormal: $\int_{-\infty}^{\infty} \psi_i^*(x)\psi_j = \delta_{i,j}$

Example: The infinite square well

The most simple potential:

$$V(x) = \begin{cases} = V_0 & \text{if } 0 < x < L \\ = \infty & \text{at } x = 0 \text{ and } x = L \end{cases}$$

Wavefunction $\psi(x)$ has to vanish at $x = 0$ and $x = L$ and obey Schrödinger equation:

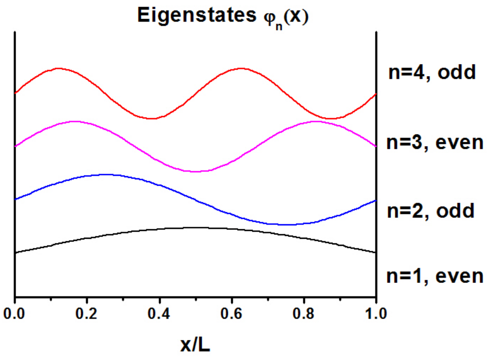
$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin(k_n x) \text{ where } k_n = n\pi/L \text{ for } n = 1, 2, \cdots$$

Substituting back into Schrödinger equation we obtain the energy Eigenvalues:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} + V_0$$

Solutions of the infinite square well potentials

Since the potential is symmetric, we have even and odd parity solutions (functions are shifted vertically for clarity)



Numerically solving the Schrödinger equation

For simplicity, we put infinite wells at $x = 0$ and $x = L$, with an arbitrary potential between the wells.
First step: Non-dimensionalize the equation to avoid computations with small numbers:

$$\frac{d^2\psi(\tilde{x})}{d\tilde{x}^2} + \gamma^2 \left(\epsilon - \nu(\tilde{x})\right) \psi(\tilde{x}) = 0, \tag{2}$$

- $\tilde{x} = x/L$ is the non-dimensional spatial variable.
- $\nu(\tilde{x}) = V(\tilde{x})/V_0$: dimensionless potential energy with a range of values between -1 and $+1$.
- $\epsilon = E/V_0$ is a dimensionless energy
- $\gamma^2 = \frac{2mL^2V_0}{\hbar^2}$
- L is the physical size of the well.
- m is mass of the particle.

Numerically solving the Schrödinger equation

Equation is of the form:

$$\frac{d^2\psi}{dx^2} + k^2(x)\psi(x) = 0$$

an be integrated by the Numerov 3-point formula (see Appendix I of handout for derivation):

Numerov algorithm

$$\psi_{n+1} = \frac{2\left(1 - \frac{5}{12}l^2k_n^2\right)\psi_n - \left(1 + \frac{1}{12}l^2k_{n-1}^2\right)\psi_{n-1}}{1 + \frac{1}{12}l^2k_{n+1}^2},$$

where l is the integration step size: $l \equiv x_{i+1} - x_i = 1/(N-1)$ for N evaluation points.

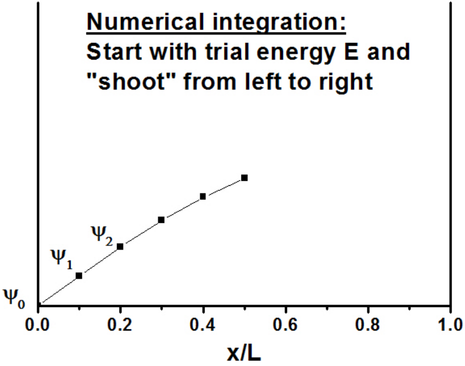
By specifying two neighbouring points, one can obtain the third point.

For the Schrödinger equation,

$$k_n^2 = \gamma^2\left(\epsilon - \nu(x_n)\right)$$

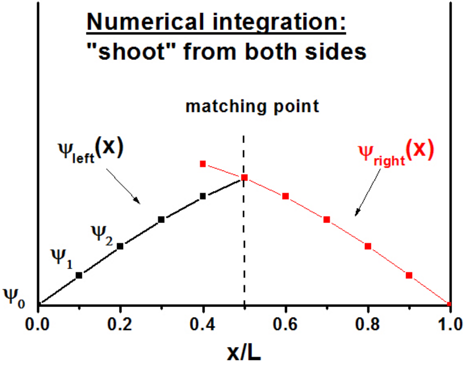
Numerically solving the Schrödinger equation

Now we can apply this algorithm to the infinite square well potential: We know that $\psi(\tilde{x})$ vanishes at both sides of the well: $\psi(\tilde{x}=0)=\psi(\tilde{x}=1)$
Let $x_n = n \cdot l$, where $n = 0 \cdots N-1$ and $l = 1/(N-1)$.
NOTE: $\psi(x_1)$ is arbitrary!



Numerically solving the Schrödinger equation

Now shoot from both sides. Matching point is in the middle. Due to the symmetry of the potential, $\psi_{left}(x)$ and $\psi_{right}(x)$ will meet in the middle. But slopes are discontinuous unless you have an energy Eigenstate.



Asymmetric potentials

- Main task will be to write a routine that finds the energy Eigenstate that will minimize the difference in the slopes.
- Later on will look at an asymmetric potential. $\psi_{left}(x)$ and $\psi_{right}(x)$ will not meet at the matching point.
- Need to rescale either $\psi_{left}(x)$ or $\psi_{right}(x)$, such that $\psi_{left}(x_{match}) = \psi_{right}(x_{match})$.
- We are allowed to do that! Even though the $\psi(x)$'s may not satisfy the boundary condition, they still satisfy the Schrödinger equation. Therefore, we can multiply the wave function by any constant.
- After rescaling, you can apply the same procedure to make the slopes continuous and thereby find the energy Eigenstate.

Template

- Don't worry! You will start from a template that does the integration from both sides for a given trial energy.
- Details about the source code and the Numerov algorithm can be found in the handout.
- Read the code carefully and ask me or Steven Tobin if you are stuck.
- Play around and enjoy!
- This introduction, the handout with what you have to do and the template can be found:

`http://www.tcd.ie/Physics/People/Matthias.Moebius/teaching/`